

Kinky Behavior in Josephson Junctions

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We analyze nonperturbatively the behavior of a Josephson junction in which two BCS superconductors are coupled through an Anderson impurity. We recover earlier perturbative results which found that a $\delta = \pi$ phase difference is preferred when the impurity is singly occupied and the on-site Coulomb interaction is large. We find a novel intermediate phase in which one of $\delta = 0$ and $\delta = \pi$ is stable while the other is metastable, with the energy $E(\delta)$ having a kink somewhere in between. As a consequence of the kink, the $I - V$ characteristics of the junction are modified at low voltages.

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I. INTRODUCTION

Two identical superconductors separated by a barrier will generate a Josephson current $J(\delta) = J_c \sin(\delta)$, where δ is the phase difference between the superconductors. J_c is given by the Ambegaokar-Baratoff formula $J_c = \pi\Delta/2eR$, where Δ is the superconducting gap and R is the normal state resistance of the barrier. This result is derived perturbatively, assuming some (spin-conserving) tunneling amplitude t for electrons to move across the barrier region; the conductance $G = 1/R$ is then proportional to $|t|^2$ when t is small. In the 1960's, Kulik [1] showed that tunneling processes which do not conserve spin act to decrease J_c and potentially drive it negative, so that $J_c \propto |t|^2 - |t_{sf}|^2$, where t_{sf} is the amplitude for spin flip tunneling across the barrier.

This result was generalized to the case of tunneling through a dynamical (Kondo or Anderson) impurity by Shiba and Soda [2] and by Glazman and Matveev [3]. The essence of negative Josephson coupling was also elucidated by Spivak and Kivelson [4], who considered an interacting barrier region comprised of a single Anderson impurity. Assuming the local Hubbard U is large and the impurity is singly occupied, they showed that the fourth order process

SC #1	IMPURITY	SC #2
$\uparrow\downarrow$	\uparrow	$-$
$\uparrow\downarrow$	$-$	\uparrow
\uparrow	\downarrow	\uparrow
\uparrow	$-$	$\downarrow\uparrow$
$-$	\uparrow	$\downarrow\uparrow$

reverses the order of spins in the Cooper pair, and hence leads to a negative Josephson coupling. For an Anderson impurity with site energy ε_0 , the condition for single occupancy (for infinitesimal hopping) is $U > -\varepsilon_0 > 0$.

When $J_c < 0$, the most favorable configuration for the junction is one in which the phase difference is $\delta = \pi$. In

a ring with a single such π -junction, time reversal is broken and there is a trapped flux of $\pm hc/4e$ [5]. In recent years, several experiments [6] have focussed on the existence of π -junctions in high T_c superconductors and have been invoked as evidence for the existence of a $d_{x^2-y^2}$ wave order parameter therein.

In this paper, we are again concerned with simple s -wave superconductors coupled via an Anderson impurity. We rederive earlier results on π -junctions using nonperturbative techniques, and we find a crossover region, which separates 0- and π -junction behavior. This crossover regime is characterized by a ground state energy $E(\delta)$ which has local minima at both $\delta = 0$ and $\delta = \pi$, and a kink at its maximum, occurring at an intermediate value of δ . We derive a phase diagram as a function of $-\varepsilon_0/\Delta$, U/Δ , and Γ/Δ , where Γ is the bare impurity level width generated by virtual hopping onto the superconductors. We also discuss the $I(V)$ behavior of such a junction within the resistively shunted junction (RSJ) model.

II. EFFECTIVE ACTION

Consider two superconducting planes each of which is connected via electron hopping to an Anderson impurity. For electrons living in a fully two-dimensional space, the field operator $\psi(\mathbf{r})$ may be decomposed into partial waves [7,8],

$$\psi^\dagger(\mathbf{r}) = \sum_{l=-\infty}^{\infty} e^{il\phi} \int_0^{\infty} \frac{dk}{2\pi} \sqrt{k} J_l(kr) \psi_l^\dagger(k) \quad (1)$$

where $\{\psi_l(k), \psi_{l'}^\dagger(k')\} = 2\pi \delta_{ll'} \delta(k - k')$ and where spin indices have been suppressed. Within each l sector, the kinetic energy can be linearized to $\varepsilon \simeq \hbar v_F(k - k_F)$. Extending the lower limit of k from 0 to $-\infty$ is innocuous provided we are interested in low energy properties which only involve states for which $|k - k_F| \ll k_F$. Each l sector,

then, yields a single chiral fermion branch on the real line (or two chiral fermions on a half line):

$$\psi_l^\dagger(x) \equiv \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \psi_l^\dagger(k)$$

$$\mathcal{T}_l = \hbar v_F \int_{-\infty}^{\infty} dx \psi_l^\dagger(x) \left(\frac{1}{i} \frac{\partial}{\partial x} - k_F \right) \psi_l(x). \quad (2)$$

Since $\psi(\mathbf{0}) \simeq \sqrt{k_F} \psi_{l=0}(0)$, so only the $l = 0$ channel is involved in connecting the two planes.

Modeling the superconductors with the BCS Hamiltonian, we make use of

$$\int d^2r \psi_\uparrow^\dagger(\mathbf{r}) \psi_\downarrow^\dagger(\mathbf{r}) = \int_0^\infty \frac{dk}{2\pi} \sum_l (-1)^l \psi_{l\uparrow}^\dagger(k) \psi_{-l\downarrow}^\dagger(k)$$

$$\simeq \sum_l (-1)^l \int_0^\infty dx \psi_{l\uparrow}^\dagger(x) \psi_{-l\downarrow}^\dagger(-x), \quad (3)$$

which is nonlocal in this representation. It may be rendered local by means of the canonical transformation $\psi_\uparrow^\dagger(x) \rightarrow \psi_\uparrow^\dagger(-x)$, which converts up spins into left movers. We now integrate out the Fermi fields at all points other than $x = 0$; this means that only the $l = 0$ modes contribute. Defining $\psi_\sigma^\dagger(\tau) \equiv \psi_{l=0,\sigma}^\dagger(x = 0, \tau)$, we obtain the effective action for the point $x = 0$,

$$S_{\text{eff}} = \sum_{\omega_m} \bar{\psi}_i(\omega_m) R_{ij}(\omega_m) \psi_j(\omega_m) \quad (4)$$

where

$$\psi_i(\omega_m) = \begin{pmatrix} \psi_\uparrow(\omega_m) \\ \bar{\psi}_\downarrow(-\omega_m) \end{pmatrix}$$

$$R_{ij}(\omega_m) = \frac{2v_F}{\sqrt{\omega_m^2 + \Delta^2}} \begin{pmatrix} -i\omega_m & \Delta e^{i\delta} \\ \Delta e^{-i\delta} & -i\omega_m \end{pmatrix} \quad (5)$$

Here, $\omega_m = 2\pi(m + \frac{1}{2})T$ is a fermionic Matsubara frequency, $\{\psi_\sigma, \bar{\psi}_\sigma\}$ are Grassmann fields, and δ is the phase of the superconducting condensate (Δ is real).

The superconductor is thus reduced the zero-dimensional action of equation (5). The on-site interactions of the Anderson impurity and its coupling to the superconductors is described by the Hamiltonian [9]

$$\mathcal{H}_1 = -\frac{t}{\sqrt{k_F}} \sum_\sigma (\psi_\sigma^\dagger c_\sigma + c_\sigma^\dagger \psi_\sigma) + \varepsilon_0 \sum_\sigma c_\sigma^\dagger c_\sigma$$

$$+ U c_\uparrow^\dagger c_\downarrow^\dagger c_\downarrow c_\uparrow. \quad (6)$$

When $t = 0$, the ground state of the impurity is singly occupied provided $U > -\varepsilon_0 > 0$. We couple the Anderson impurity to two superconductors, assumed identical

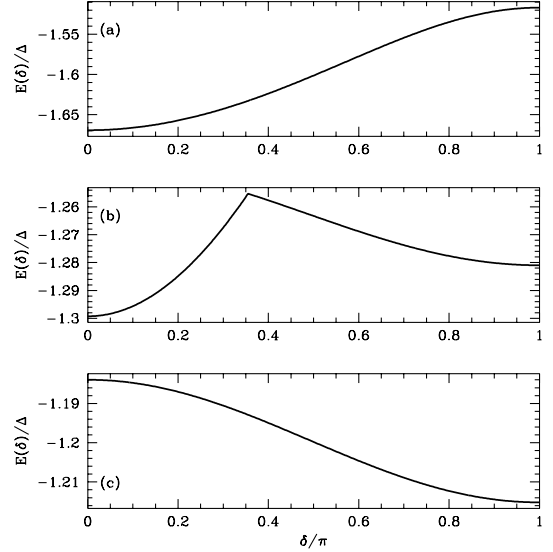


FIG. 1. Ground state energy for junctions with $\varepsilon_0 = -2$, $\Gamma/\Delta = 1$, and (a) $U = 2.1$, (b) $U = 2.6$, and (c) $U = 2.9$.

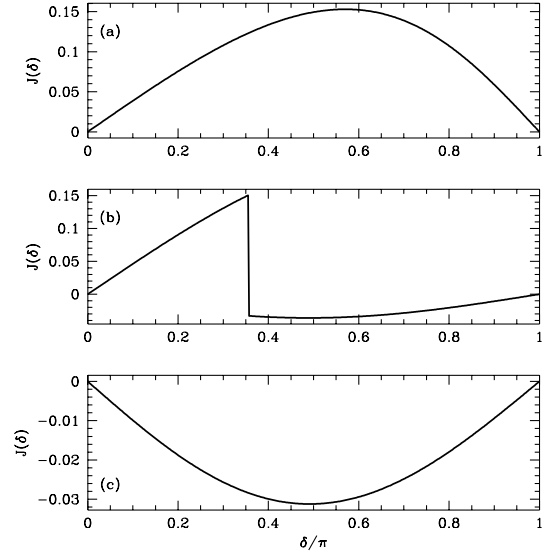


FIG. 2. Josephson current (in units of $2e\Delta/\hbar$) for junctions with $\varepsilon_0 = -2$, $\Gamma/\Delta = 1$, and (a) $U = 2.1$, (b) $U = 2.6$, and (c) $U = 2.9$.

in every respect except in their phase. We may then integrate out the $\{\psi_\sigma, \bar{\psi}_\sigma\}$ fields on each superconductor and decouple the interaction term via a Hubbard-Stratonovich (HS) transformation. Neglecting temporal fluctuations in the HS field, we have

$$Z = \frac{1}{\sqrt{2\pi UT}} \int_{-\infty}^{\infty} d\gamma \exp \left(-\frac{\gamma^2}{2UT} - \frac{\tilde{\varepsilon}_0}{T} \right) \prod_{\omega_m} \det M(\omega_m), \quad (7)$$

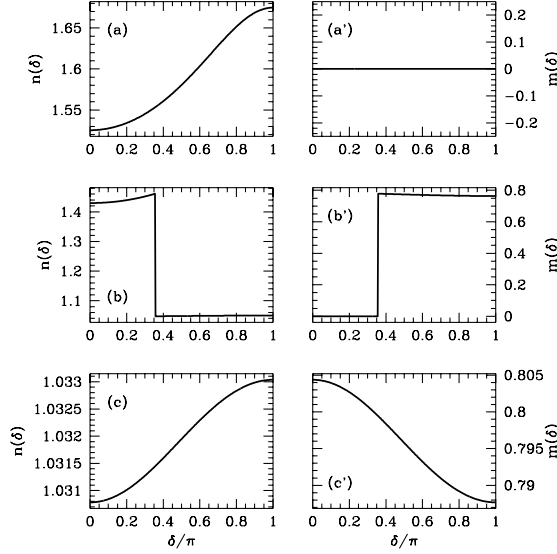


FIG. 3. Occupation number n and magnetization $m = \gamma^*/U$ for a junction with $\varepsilon_0 = -2$, $\Gamma/\Delta = 1$, and (a,a') $U = 2.1$, (b,b') $U = 2.6$, and (c,c') $U = 2.9$.

where $M(\omega_m)$ is the matrix

$$\begin{pmatrix} -i\omega_m(1 + \alpha_m) + \tilde{\varepsilon}_0 + \gamma & -\alpha_m \Delta \cos(\delta/2) \\ -\alpha_m \Delta \cos(\delta/2) & -i\omega_m(1 + \alpha_m) - \tilde{\varepsilon}_0 + \gamma \end{pmatrix},$$

where $\alpha_m \equiv \alpha(\omega_m) \equiv \Gamma/\sqrt{\omega_m^2 + \Delta^2}$ and $\Gamma = t^2/k_F v_F$ is the (bare) impurity level width. $\delta = \delta_1 - \delta_2$ is the phase difference between the two superconductors, and $\tilde{\varepsilon}_0 = \varepsilon_0 + \frac{1}{2}U$. We now make an approximation by performing the integral in (7) using the method of steepest descents. That is, we compute the free energy

$$F = -T \sum_{\omega_m} \ln \left([\omega_m(1 + \alpha_m) + i\gamma]^2 + \tilde{\varepsilon}_0^2 + [\alpha_m \Delta \cos(\frac{1}{2}\delta)]^2 \right) + \frac{\gamma^2}{2U} + \tilde{\varepsilon}_0, \quad (8)$$

and minimize over γ . We remark that this procedure is exact in the large- N limit of an $\text{Sp}(2N)$ model in which, for each \uparrow and \downarrow internal degree of freedom there are N flavors $a = 1, \dots, N$. The on-site interaction term for this model is

$$\mathcal{H}_{1,\text{int}} = -\frac{U}{2N} \sum_{a,b} (c_{a\uparrow}^\dagger c_{a\uparrow} - c_{a\downarrow}^\dagger c_{a\downarrow})(c_{b\uparrow}^\dagger c_{b\uparrow} - c_{b\downarrow}^\dagger c_{b\downarrow}) + \frac{U}{2N} \sum_{a,\sigma} c_{a\sigma}^\dagger c_{a\sigma}. \quad (9)$$

The free energy in (8) is then the free energy per flavor, and $\tilde{\varepsilon}_0 = \varepsilon_0 + (U/2N)$.

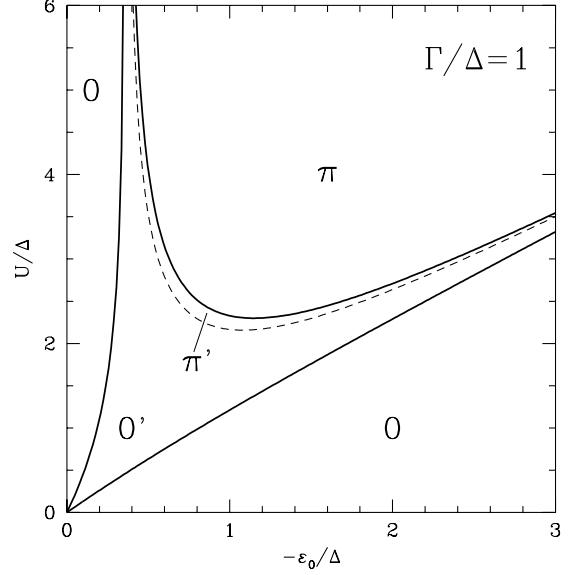


FIG. 4. The phase diagram for $\Gamma/\Delta = 1.0$. In the **0** phase (which includes all $\varepsilon_0 > 0$ as well), $\delta = 0$ minimizes the energy of the junction and $\delta = \pi$ is unstable. In the π phase, $\delta = \pi$ minimizes the junction energy and $\delta = 0$ is unstable. In the **0'** phase, $\delta = 0$ is the stable minimum while $\delta = \pi$ is metastable, and *vice versa* for the π' phase.

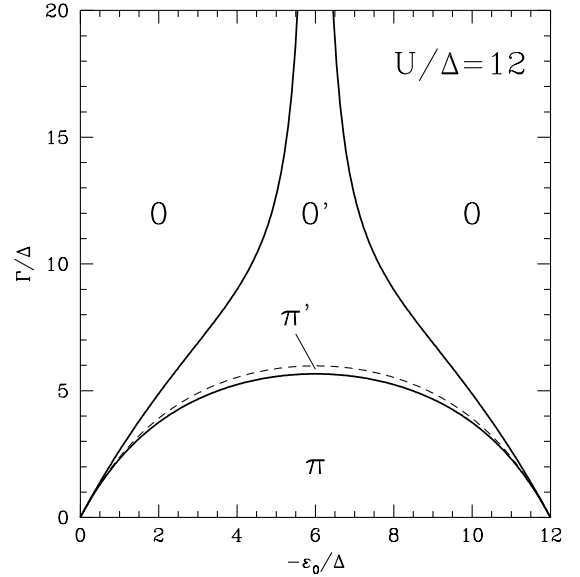


FIG. 5. The phase diagram for $U/\Delta = 12$. The phases **0**, **0'**, π , and π' are as in FIG. 4.

III. SOLUTION OF THE MODEL

At $T = 0$, the self-consistent equation for γ is

$$\frac{\partial E}{\partial \gamma^2} = \frac{1}{2U} - \int_0^\infty \frac{d\omega}{\pi} \frac{2\omega^2[1 + \alpha(\omega)]^2 A(\omega)}{A^2(\omega) + 4\gamma^2\omega^2[1 + \alpha(\omega)]^2} = 0$$

$$A(\omega) = \omega^2[1 + \alpha(\omega)]^2 - \gamma^2 + \tilde{\varepsilon}_0^2 + \alpha^2(\omega)\Delta^2 \cos^2(\frac{1}{2}\delta) \quad (10)$$

Once the solution $\gamma = \gamma^*$ is obtained, we compute the current $J = \partial E / \partial \delta$ and the impurity occupancy $n = \partial E / \partial \tilde{\varepsilon}_0$,

$$J = \int_0^\infty \frac{d\omega}{\pi} \frac{A(\omega) \alpha^2(\omega) \Delta^2 \sin(\delta)}{A^2(\omega) + 4\gamma^2 \omega^2 [1 + \alpha(\omega)]^2} \quad (11)$$

$$n = 1 - \int_0^\infty \frac{d\omega}{\pi} \frac{\tilde{\varepsilon}_0 A(\omega)}{A^2(\omega) + 4\gamma^2 \omega^2 [1 + \alpha(\omega)]^2} . \quad (12)$$

In the event that there is more than one solution for γ^* , we choose the solution with the lowest energy.

In FIGs. 1, 2, and 3 we show the mean field solution as we tune through a critical region of interaction strength U . For low U the junction is unremarkable, with $J(\delta) \approx J_c \sin(\delta)$ and $J_c > 0$. (The deviation from a pure $\sin(\delta)$ behavior occurs because $\Gamma/\Delta = 1$ is not so small.) The energy $E(\delta)$ exhibits a minimum at $\delta = 0$, and the curve $n(\delta)$ shows that the Anderson impurity is compressible in that the occupancy responds to changes in δ . At high U , the behavior is inverted: $J_c < 0$ and $E(\delta)$ has a minimum at $\delta = \pi$. The occupancy of the Anderson impurity is effectively pinned – the impurity is incompressible. This is the regime discussed by Spivak and Kivelson – for $\varepsilon_0 < 0$ and U sufficiently large, the impurity maintains single occupancy and the fourth order process (in t) which transfers a Cooper pair from one superconductor to the other through the impurity reverses the order of the up and down spins, thereby leading to a negative Josephson coupling.

The intermediate U regime shown in the (b) panels of FIGs. 1, 2, and 3 exhibits unusual behavior. Rather than the amplitude of J_c smoothly going through zero, we find that for $\delta \in [0, \delta_c]$ the impurity is compressible and $J(\delta) > 0$, but further increase of δ results in an incompressible impurity and a reversal of the Josephson current. For the parameters given, $E(\delta)$ has a global minimum at $\delta = 0$ and a local minimum at $\delta = \pi$; the relative positions of the minima will switch at a somewhat higher value of U .

A related result was derived in Ref. [10], where the Josephson tunneling through a ferromagnet was studied. The Josephson current was obtained as a sum of partial contributions due to Andreev bound states in barrier region. Certain bound states were found to produce an anomalous phase dependence of the energy, similar to that found here.

The phase diagram for $\Gamma/\Delta = 1$ is shown in FIG. 4. In the phases marked **0** and π , the only stable minima in $E(\delta)$ lie at $\delta = 0$ and $\delta = \pi$, respectively. In the intermediate regime, both $\delta = 0$ and $\delta = \pi$ are local

minima; the global minima then label the phases **0'** and π' . We have found that the qualitative shape of this phase diagram is valid for all Γ/Δ we explored. The phase diagram in the $(-\varepsilon_0/\Delta, \Gamma/\Delta)$ plane is shown in FIG. 5. The fact that the **0'** phase persists in an ever-narrowing region about $\varepsilon_0 = -\frac{1}{2}U$ is an artifact of the large- N model, which is unable to describe the Kondo physics which sets in below temperatures on the order of $T_K \sim \Gamma \exp(-\pi|\varepsilon_0|/2\Gamma)$ [3]. The solid lines in FIGs. 4 and 5, all represent first order transitions, where all quantities (n , J , m , *etc.*) are discontinuous.

There is a symmetry in our model under $\tilde{\varepsilon}_0 \rightarrow -\tilde{\varepsilon}_0$, *i.e.* $-\varepsilon_0 \rightarrow U + \varepsilon_0$, as is evident in FIG. 5. The phase boundaries in the lower left corner all start out linearly with the same slope, which may be determined via evaluating the energy shifts of the impurity states $|0\rangle$ and $|\uparrow\rangle$ doing perturbation theory in the hopping t . This line is determined to $\mathcal{O}(\Gamma)$ by $E_{|0\rangle} = E_{|\uparrow\rangle}$, which gives

$$-\varepsilon_0 = \frac{\Gamma}{4\pi} \frac{U}{\sqrt{U^2 - \Delta^2}} \ln \left(\frac{U + \Delta + \sqrt{U^2 - \Delta^2}}{U + \Delta - \sqrt{U^2 - \Delta^2}} \right) . \quad (13)$$

This gives a slope $d\Gamma/d(-\varepsilon_0)$ which depends on U/Δ . Our large- N theory tends to underestimate this slope.

How might a cusp in $E(\delta)$ manifest itself in an experiment on a single junction? Within the RSJ model, we have for $I > I_c$ that the average voltage \bar{V} across the junction is

$$\bar{V} = R \int_0^{2\pi} \frac{d\delta}{2\pi} \left[I - \frac{2e}{\hbar} \frac{\partial E}{\partial \delta} \right]^{-1} . \quad (14)$$

For a simple model of the **0'** or π' phase, we take

$$E(\delta) = \begin{cases} (\hbar/4e)I_0\delta^2 & \text{if } 0 \leq \delta \leq \delta_c \\ E_\pi + (\hbar/4e)I_1(\delta - \pi)^2 & \text{if } \delta_c \leq \delta \leq 2\pi - \delta_c \\ (\hbar/4e)I_0(\delta - 2\pi)^2 & \text{if } 2\pi - \delta_c \leq \delta \leq 2\pi \end{cases}$$

where I_0 , I_1 , δ_c , and E_π are related through continuity of $E(\delta)$ at $\delta = \delta_c$, the location of the cusp. The function $I(\bar{V})$ is shown in Fig. 6. The textbook result, when $E = E_0(1 - \cos \delta)$, is $I = \sqrt{I_c^2 + (\bar{V}/R)^2}$. In our model, the cusp results in a much flatter behavior as $\bar{V} \rightarrow 0$, with

$$I(\bar{V}) = I_c + \lambda I_c \exp(-V_0/\bar{V}) \quad (15)$$

where $I_c = \max((\delta_c/\pi) \cdot I_0, (1 - \delta_c/\pi) \cdot I_1)$, and λ and V_0 are constants.

It has been brought to our attention that two conventional Josephson junctions in series will also yield a kink

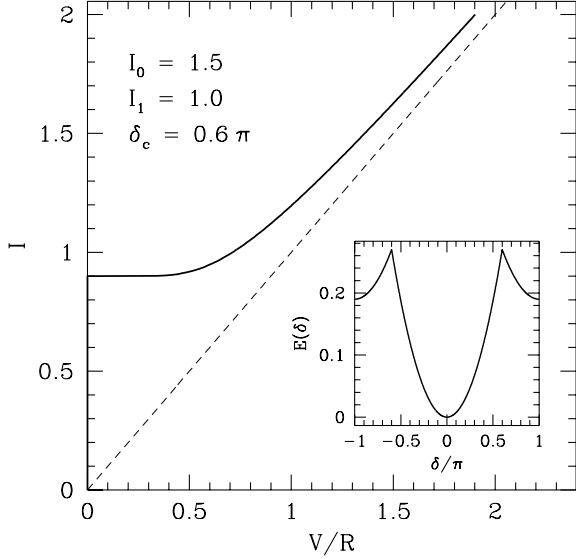


FIG. 6. I - V diagram for the simple analytical \mathbf{O}' junction model (see text). While qualitatively similar to the usual $I = \sqrt{I_c^2 + (\bar{V}/R)^2}$ behavior, here $I(\bar{V})$ flattens out much more rapidly as $V \rightarrow 0$. The inset shows the energy $E(\delta)$. This $I - V$ behavior also holds for π' -junctions.

in $E(\delta)$ [11]. If the junctions are identical, then at $T = 0$ each is responsible for half the total phase difference, and $E(\delta) = 2E_0(1 - |\cos(\frac{1}{2}\delta)|)$. However, if each junction is resistively shunted, then individual $V(I)$ curves simply add, and one does not obtain the behavior in (15).

IV. CONCLUSIONS

If single electron tunneling between superconductors flips the electron's spin, then a Cooper pair is transferred with opposite sign. This result, as first shown by Kulik [1], can lead to a negative Josephson coupling, in which case the ground state of the junction is one in which there is a $\delta = \pi$ phase difference between the two superconductors. This phenomenon was subsequently reconsidered [2,5,3,4], but in a richer and physically realizable context – tunneling through an Anderson impurity. When the tunneling amplitude t onto the impurity is small, the ground state is a π -junction provided that the impurity is singly occupied, *i.e.* $U > -\varepsilon_0 > 0$. We have derived the (approximate) nonperturbative phase diagram for the junction valid at finite t , and in so doing have discovered the existence of two additional phases, denoted \mathbf{O}' and π' , in which the ground state energy $E(\delta)$ has a cusp at some $\delta \in [0, \pi]$. This behavior is manifested in the $I(\bar{V})$ characteristic of the junction, where for small voltage \bar{V} the current approaches the critical current I_c extremely rapidly. It is also clear that systems with magnetic impurities should be sensitive to an external magnetic field.

However, tunneling experiments reported in [12] demonstrated the absence of such dependence up to fields of 6 T. This could be explained by an antiferromagnetic interaction between the impurity sites, a possibility we are now investigating.

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V. APPENDIX A

In this appendix we discuss some subtleties associated with the Hubbard-Stratonovich transformation for interacting fermions. Suppose $\gamma(\tau)$ is distributed according to

$$P[\gamma(\tau)] = \mathcal{N} \exp \left(-\frac{1}{2U} \int_0^\beta d\tau \gamma^2(\tau) \right) \quad (16)$$

where \mathcal{N} normalizes the distribution. Then averaging with respect to $P[\gamma(\tau)]$ one finds, for $M(\tau)$ a commuting variable,

$$\left\langle \exp \left(-\int_0^\beta d\tau \gamma(\tau) M(\tau) \right) \right\rangle = \exp \left(\frac{U}{2} \int_0^\beta d\tau M^2(\tau) \right).$$

Now consider the simplest Hamiltonian imaginable – a single spinless fermion with $\mathcal{H}_a = -\mu c^\dagger c$. We compute the partition function via a coherent state path integral, and since if we let $M(\tau) = \bar{c}(\tau) c(\tau)$, then from $M^2(\tau) = 0$ we obtain the result

$$\begin{aligned} Z_a &= \left\langle \int \mathcal{D}[\bar{c}, c] \exp \left(-\int_0^\beta d\tau \bar{c}(\partial_\tau + \gamma(\tau) - \mu) c(\tau) \right) \right\rangle \\ &= \left\langle \det (\partial_\tau + \gamma(\tau) - \mu) \right\rangle \\ &= \left\langle 1 + \exp \left(\beta\mu - \int_0^\beta d\tau \gamma(\tau) \right) \right\rangle \\ &= 1 + e^{\mu/T} e^{U/2T} \end{aligned} \quad (17)$$

which is incorrect – the $e^{U/2T}$ factor should not be present in the second term.

If we consider another trivial model,

$$\mathcal{H}_b = -\mu(c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow) + U c_\uparrow^\dagger c_\downarrow^\dagger c_\downarrow c_\uparrow \quad (18)$$

and let $M(\tau) = \bar{c}_\uparrow c_\uparrow - \bar{c}_\downarrow c_\downarrow$, we again obtain an incorrect result,

$$Z_b = 1 + 2 e^{\mu/T} e^{U/2T} + e^{2\mu/T} . \quad (19)$$

These problems do not appear in the discrete time version of the fermionic path integral. The discrete action is, for spinless fermions,

$$S_{\text{discrete}} = \sum_{i,j}^N \bar{c}_i M_{ij} c_j \quad (20)$$

where $N = \beta/\epsilon$ is the number of time slices, and, for \mathcal{H}_a , the matrix M_{ij} is

$$\begin{pmatrix} 1 & 0 & \cdots & 1 - \epsilon\tilde{\gamma}_N \\ -1 + \epsilon\tilde{\gamma}_1 & 1 & 0 & 0 \\ 0 & -1 + \epsilon\tilde{\gamma}_2 & 1 & \vdots \\ \vdots & & & 0 \\ 0 & \cdots & 0 & -1 + \epsilon\tilde{\gamma}_{N-1} & 1 \end{pmatrix}$$

where $\tilde{\gamma}_n \equiv \gamma_n - \mu$. We must now integrate out the Grassmann variables and then average over the distributions

$$P(\gamma_j) = \left(\frac{\epsilon}{2\pi U} \right)^{1/2} \exp(-\epsilon\gamma_j^2/2U)$$

for each time slice j . But now we find

$$\det M = 1 + \prod_{j=1}^N (1 - \epsilon\gamma_j + \epsilon\mu) \quad (21)$$

and indeed

$$\begin{aligned} Z_a &= \langle \det M(\gamma_1, \dots, \gamma_N) \rangle_{\{\gamma_i\}} \\ &= 1 + (1 + \epsilon\mu)^N \\ &= 1 + e^{\mu/T} . \end{aligned} \quad (22)$$

When we apply the discrete time path integral to \mathcal{H}_b , we find

$$\begin{aligned} \det M_{\uparrow} \det M_{\downarrow} &= 1 + \prod_{j=1}^N (1 - \epsilon\gamma_j + \epsilon\mu) + \prod_{j=1}^N (1 + \epsilon\gamma_j + \epsilon\mu) \\ &\quad + \prod_{j=1}^N ((1 + \epsilon\mu)^2 - \epsilon^2\gamma_j^2) \end{aligned} \quad (23)$$

and we find, correctly,

$$Z_b = 1 + 2 e^{\mu/T} + e^{(2\mu-U)/T} . \quad (24)$$

The essence of the problem is that in the discrete case we have

$$\langle 1 - \epsilon\gamma_j \rangle = 1$$

whereas if we write $1 - \epsilon\gamma \approx \exp(-\epsilon\gamma)$ and then average,

$$\langle \exp(-\epsilon\gamma_j) \rangle = \exp\left(\frac{1}{2}\epsilon U\right) ,$$

which gives an incorrect contribution at $\mathcal{O}(\epsilon)$.

The remedy for this frustrating problem is to perform a shift

$$\mu \rightarrow \tilde{\mu} \equiv \mu - \frac{1}{2}U \quad (25)$$

in the continuum case. This rescues the correct results from both equations (17) and (19), and may be formally obtained by point splitting $M^2(\tau) \rightarrow M(\tau^+) M(\tau^-)$.

VI. APPENDIX B

To demonstrate the reliability of the formalism and approximations used in this paper, we consider the toy model

$$\mathcal{H}_c = -\mu(c_{\uparrow}^{\dagger}c_{\uparrow} + c_{\downarrow}^{\dagger}c_{\downarrow}) + \Delta(c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger} + c_{\downarrow}c_{\uparrow}) + U c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}c_{\downarrow}c_{\uparrow} .$$

Once again we break up the interaction term with a Hubbard-Stratonovich transformation, careful to substitute $\mu \rightarrow \tilde{\mu}$. All the time dependence of the field $\gamma(\tau)$ can be gauged away via the transformation

$$\begin{aligned} c(\tau) &\rightarrow e^{-g(\tau)} c(\tau) \\ \partial_{\tau} g(\tau) &= \gamma(\tau) - \frac{1}{\beta} \int_0^{\beta} d\tau' \gamma(\tau') . \end{aligned} \quad (26)$$

Note that $g(\beta) = g(0)$, so the antiperiodic boundary conditions $c(\beta) = -c(0)$ are not affected by this transformation. Thus,

$$\begin{aligned} Z_c &= \frac{1}{\sqrt{2\pi U T}} \int_{-\infty}^{\infty} d\gamma e^{-\gamma^2/2UT} e^{(\tilde{\mu}+\gamma)/T} \\ &\quad \times \det \begin{pmatrix} \partial_{\tau} + \gamma - \tilde{\mu} & \Delta \\ \Delta & \partial_{\tau} + \gamma + \tilde{\mu} \end{pmatrix} , \end{aligned} \quad (27)$$

where now γ is time-independent, denoting simply the average of what we have until now been calling the function $\gamma(\tau)$. Now if $\{\lambda_0, \dots, \lambda_3\}$ are constants, then

$$\det(\partial_{\tau} + \lambda_0 + \vec{\lambda} \cdot \vec{\sigma}) = 1 + 2 e^{-\lambda_0/T} \cosh \frac{|\vec{\lambda}|}{T} + e^{-2\lambda_0/T} . \quad (28)$$

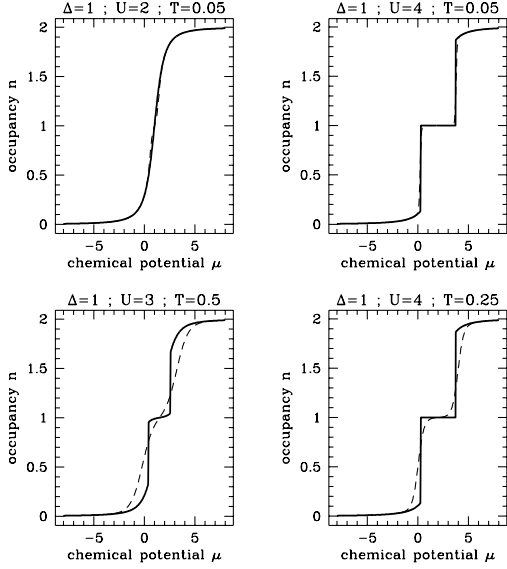


FIG. 7. Occupancy n versus bare chemical potential μ for the toy model \mathcal{H}_c computed in the steepest descents approximation (solid) and compared with exact results (dashed).

Performing the integral over γ , one correctly obtains the partition function which may be calculated by more elementary means.

The steepest descents approximation (SDA) to the integral over γ gives

$$\frac{\gamma}{U} = \frac{1 - e^{-2\gamma/T}}{1 + 2e^{-\gamma/T} \cosh \frac{\sqrt{\tilde{\mu}^2 + \Delta^2}}{T} + e^{-2\gamma/T}}, \quad (29)$$

which is obtained by extremizing

$$F = \frac{\gamma^2}{2U} - \gamma - \tilde{\mu} - T \ln \left(1 + e^{-(\gamma - \sqrt{\tilde{\mu}^2 + \Delta^2})/T} \right) - T \ln \left(1 + e^{-(\gamma + \sqrt{\tilde{\mu}^2 + \Delta^2})/T} \right) \quad (30)$$

with respect to γ . $\gamma = 0$ is always a solution, and for a range of parameters it is possible to have more than one solution to (29), in which case we choose the solution with the lowest free energy. Once a solution for γ is obtained, we evaluate the particle number

$$N = -\frac{\partial F}{\partial \tilde{\mu}} \quad (31)$$

$$= 1 + \frac{\tilde{\mu}}{\sqrt{\tilde{\mu}^2 + \Delta^2}} \frac{2e^{-\gamma/T} \sinh \frac{\sqrt{\tilde{\mu}^2 + \Delta^2}}{T}}{1 + 2e^{-\gamma/T} \cosh \frac{\sqrt{\tilde{\mu}^2 + \Delta^2}}{T} + e^{-2\gamma/T}}.$$

Comparisons of the SDA with the exact results are shown in FIG. 7. For the Hamiltonian \mathcal{H}_c , the SDA is exact in the limit of zero temperatures. At finite T , the SDA leads

to isolated discontinuous changes of γ as μ , U , and Δ are varied, which are reflected in the behavior of *e.g.* $n(\mu)$. The exact solution behaves smoothly, but for sufficiently low temperatures the agreement is arbitrarily good.

VII. BIBLIOGRAPHY

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